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## **Final Progress Report**

### **Phonon kinetics and heat removal from low-dimensional semiconductor structures**

#### **Statement of the problems studied**

Our research on electron-phonon and phonon-phonon processes in low-dimensional semiconductor nanostructures has been focused on the effects of a surfaces and interfaces on the electron energy and momentum relaxation rates due to acoustic phonon emission [1-8, 11, 16-21], new specific mechanism of electron interaction with acoustic phonons in semiconductor heterostructures [9-10], electron and phonon heating [1,7, 12-14], and phonon-induced processes of charge carriers loosing phase coherence in heterostructures [4,7]. Our research provides the necessary basis for the control of the heat dissipation and for the design of nanodevices with electron-phonon relaxation rates required for specific applications, such as quantum computing [4,23], ultrasensitive hot-electron detectors and quantum nanocalorimeters [5], fast transistors, and light-emitting devices. The following briefly describes our results.

#### **Summary of the most important results**

##### ***1. Effects of Surfaces and Interfaces on Energy and Momentum Relaxation Rates***

In the first part of our study, we addressed the effect of proximity of a quantum well to a stress-free surface of the semiconductor heterostructure on the momentum relaxation rate of two-dimensional electrons interacting with acoustic phonons via piezoelectric and deformation potentials. The peculiarities of the near-surface scattering originate from two sources: modification of the acoustic-

phonon modes caused by the stress-free crystal surface and dependence of the phonon-induced piezoelectric potential on the dielectric properties of a medium ion contact with the semiconductor. The result obtained demonstrate that for narrow quantum wells placed close to the surface the relaxation rate at low temperatures (Bloch-Gruneisen regime) is changed considerably in comparison with that of a two-dimensional electron gas placed in a bulk of semiconductor. For the temperatures where the piezoelectric potential interaction dominates over the deformation potential interaction, the near-surface relaxation rate is enhanced in the case of a semiconductor-vacuum system and is suppressed in the case of the surface covered by a thin metal film. The temperature dependence of the near-surface momentum relaxation rate is found to be  $T^{-1}$  for values of the temperature  $T$  far below the Bloch-Gruneisen temperature. For a semiconductor-vacuum system,  $\alpha=3$  and  $\beta=5$  for piezoelectric and deformation potential scattering, respectively; for a semiconductor-metal system,  $\alpha=5$  for both mechanisms. The screening effects taking into account changes the temperature dependencies of momentum relaxation rates: for a semiconductor-vacuum system, the temperature dependencies are now determined by  $\alpha=7$  and also  $\beta=7$  for piezoelectric and deformation potential scattering, respectively. Surprisingly, the screening does not change the value of  $\beta$  in the case of metal-semiconductor system.

In the second part, we model the influence of a cap layer with a fixed thickness placed on top of a semi-infinite heterostructure on the energy and momentum relaxation rates for two-dimensional electrons localized in the lowest subband of a quantum well and interacting with the acoustic phonon via the deformation potential. The relaxation rates are derived from the corresponding balance equations for a small deviation from the thermodynamics equilibrium. Our numerical results indicate that at low temperatures the efficiency of the scattering is changed substantially depending on the mechanical conditions at the surface; the cases of free and rigid surfaces are considered. We have analyzed the dependencies of the electron energy and momentum rates on the distance from the electron layer to the surface, on the temperature and electron concentration. The efficiencies of relaxation are shown to change substantially (up to two times for standard parameters of GaAs or InAs based quantum wells) depending nonmonotonically on the distance of the 2D layer to the surface and on the electron temperature. Decreasing the momentum relaxation rate due to the surface effect in thin (to 5 nm width) quantum wells gives rise to the possibility of obtaining 2D electron layers with extremely high mobility, limited only by the scattering on structure defects and on roughness of the interfaces, under higher temperatures. Thus, phonon engineering may be used to substantially modify the relaxation processes in selected quantum-based devices.

We have considered the emission of nonequilibrium acoustic phonons in the process of spin-flip transitions of electrons in non-symmetric quantum wells. The spin-splitting of the electron energy spectra causes the modifications of the energy and angular distributions as functions of the transverse voltage. The spin-flip

contribution to the emission rate is substantial for the phonons being emitted at considerable angles to the normal direction. The intensity of phonon emission for such angles increases in several times for InAs-based quantum wells, due to the contribution of spin-flip transitions.

## ***2. Contribution of Effective Mass Variation to Electron Scattering on Acoustic Phonons***

In bulk semiconductors, interaction via the deformation potential is the predominant mechanisms of electron scattering on acoustic phonons. This interaction was also thought to determine the kinetics of confined electrons in quantum heterostructures, the size and shape of the heterostructure affecting only the wave functions of participating phonon modes. We have suggested and explored a new specific mechanism of electron interaction with acoustic phonons in heterostructures, which is determined by the electron effective mass variation in the structure.

We have demonstrated the role of the deformation dependence of the electron effective mass in the interaction of electrons with acoustic phonons in quantum heterostructures. Starting from microscopic consideration, we have derived the electron-acoustic phonon interaction Hamiltonian, which describes the deformation-potential interaction and the overall contribution of the interfaces. To determine the electron energy perturbation caused by a smooth lattice displacement, we used the model of deformed ions. In this approach, the presence of interfaces is accounted for by the lattice potential. To calculate the electron wave functions, we exploited a tight-binding approach in a crystal with a simple cubic lattice and assumed that only first-neighbor cell couplings are nonzero.

We have demonstrated that the interaction of electrons confined in a nanostructure with acoustic phonons in a cubic crystal is described by a deformation-potential tensor whose symmetry is determined by the geometry of the nanostructure. The deformation dependence of the effective mass contributes considerably to a size-dependent part to the electron-acoustic phonon interaction. This contribution can exceed those from the usual deformation potential and from complementary mechanism due to the vibrations of heterointerface boundaries. Unlike the usual deformation interaction in cubic crystals, the new mechanism as well as the boundary-vibration mechanism may involve electron interaction with transverse acoustic phonons. For narrow quantum wells, the interaction with longitudinal acoustic modes caused by the new mechanism is comparable to and may overcome that from the bulk deformation potential.

Having used the obtained general formulas, we considered the finite-size effect in the interlevel transitions in cubical quantum dots in a GaAs structure. The new contribution to the electron-acoustic phonon Hamiltonian which is caused by the

deformation dependence of the electron effective mass is proportional to inverse square of the quantum dot. Therefore, the obtained correction terms grow considerably with the dot size decreasing. For small GaAs-based quantum dots, this contribution is comparable with and can overcome that from the usual deformation potential coupling.

However, for small (<50nm) quantum dots our continuum approach becomes inappropriate. Thus, further development of the theory is necessary to describe small-dot structures, which are especially important in applications.

### *3. Phonon-induced Electron Dephasing in Heterostructures*

The electron dephasing in ultrathin films and nanostructures is of vital importance for nanoelectronics and has been intensively studied during recent decades. Temperature-dependent dephasing rate is mainly determined by the electron-electron and electron-phonon interactions. While theoretical results pertaining to electron-electron scattering are confirmed by many experiments, the electron-phonon mechanism is still poorly understood.

Unfortunately, most researchers employ the standard clean-limit concept, its uncritical application leading to incorrect and controversial conclusions. We suggest and investigate more reliable electron-phonon interaction model taking into account electron scattering from boundaries, defects and impurities. We found that even relatively weak static potential drastically changes the effective electron-phonon coupling and corresponding electron dephasing rate.

The electron scattering from boundaries and impurities destroys the single-particle picture of the electron-phonon interaction. We have shown that quantum interference between 'pure' electron-phonon and electron-boundary/impurity scattering may result in the reduction as well as to the significant enhancement of the electron dephasing rate. This effect crucially depends on the extent to which electron scatterers, such as boundaries and impurities, are dragged by phonons.

In our model [1,7], both static and vibrating scatterers are described by two dimensionless parameters  $ql$  and  $qL$ , where  $q$  is the wave vector of the thermal phonon,  $l$  is the total electron mean free path, and  $L$  is the mean free path due to scattering from static scatterers. Without static scatterers, the dephasing rate at low temperatures is slower by the factor  $1/ql$  than the rate in a pure bulk material. In contrast, in the presence of static potential the dephasing becomes  $1/qL$  times faster. This low-temperature electron dephasing is mainly determined by transverse phonons.

Thus, at low temperatures electron dephasing and energy relaxation may be controlled by electron boundary/impurity scattering in a wide range, which is

apparently important for applications. The dephasing rate can be increased or decreased compared to the rate in a pure bulk material. The predicted enhancement of the electron-phonon interaction due to disorder and  $T^{-1}$ -dependence of the electron-phonon dephasing rate have been found recently in experiments on thin metallic films and semiconducting heterostructures. In the next year, we plan to continue investigations in this direction with improved theoretical model incorporating modification of the phonon spectrum.

#### ***4. Impact on Solid-State Elements for Quantum Computing***

Study of the electron-phonon interaction in nanostructures will also have immediate impact on the design of solid-state elements for quantum computing and cryptography [4, 23, 24]. The electron-phonon interaction plays a twofold role in solid-state elements for quantum computing. In coherent boxes, it controls the dephasing of electron subsystem and limits the time, which may be used for quantum manipulation. In readout nanodevices, the electron-phonon interaction is a basic mechanism of electron relaxation, it determines the characteristic time and sensitivity of quantum electrometers. The requirements on coupling between the coherent box and environment during quantum manipulations and quantum measurements contradict each other. During manipulations, decoherence should be minimized, while during measurements the quantum state should be dephased. To provide dephasing, the quantum measurement is performed by driving the electrometer out of equilibrium. After nonequilibrium dephasing the electrometer should relax to equilibrium as fast as possible.

The problem of the fast electron-phonon relaxation after quantum measurement is even more important. The increase of electron-phonon scattering time with decreasing operating temperature is very significant: it causes a very large thermal resistance between electrons and phonons. As a result, electrons are easily overheated by an external disturbance and slowly relax to equilibrium. For instance, at an operating temperature of 25mK and a bias current of  $I=5\text{pA}$  via the electrometer, the effective temperature was found to be 220mK (see [4,23]). At an operating temperature of 20 mK the effective electron temperature was determined to be about 80mK. Thus, as emphasized slow electron-phonon relaxation limits applications of solid-state elements at ultralow temperatures.

Our research allows one to control the electron-phonon relaxation and dephasing rates in nanostructures, which are considered as promising elements for quantum computing.

#### **6. List of all publications and technical reports supported under this grant.**

*Papers published in peer-reviewed journals:*

1. "Breakdown of Pippard Ineffectiveness Condition for Phonon-electron Scattering in Micro and Nanostructures", A. Sergeev and V. Mitin, Europhysics



Letters, 2000, Vol. 51, No. 6, pp. 641-647.

1. "Energy Losses of 2D Electron Gas Due to Near-Surface Acoustic Phonon Scattering", V.I. Pipa, N.Z. Vagidov, V. V. Mitin, and M. Strosio, *Supperlattices and Microstructures*, 2000, Vol. 27, No. 5/6, pp. 425-429.
1. "The Emission of Acoustic Phonons due to Spin-Flip Electron Transitions in Non-symmetric Quantum Wells", F.T. Vasko and V.V. Mitin, *Phys. Rev. B.*, 2000, Vol. 61, No. 16, pp. 11047-11050.
1. "Effect of Boundaries and Impurities on Electron-Phonon Dephasing", A. Sergeev and V. Mitin, *Supperlattices and Microstructures*, 2000, Vol. 27, No. 5/6, pp. 499-504.
1. "Photon-noise limited direct detector based on disorder controlled electron heating", B. Karasik, W.R. McGrath, M.E. Gershenson, and A.V. Sergeev, *J. Appl. Phys.*, 2000, Vol. 87, pp. 7586-7588.
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1. "Electron-Phonon Interaction in Disordered Conductors: Static and Vibrating Scattering Potentials", A. Sergeev and V. Mitin, *Phys. Rev. B.*, 2000, Vol. 61, No. 9, pp. 6041-6047.
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1. "Energy and Momentum Relaxation of Two-Dimensional Electron Gas Due to Near Surface Deformation Scattering", V. I. Pipa, F. T. Vasko, and V. V. Mitin, *J. Appl. Phys.*, 1999, vol. 85, No.5, pp. 2754-2762.
1. "Hot-Optical-Phonon Effects on Electron Relaxation in an AlGaAs/GaAs Quantum Cascade Laser Structure", G. Paulavicius, V. Mitin, and M. Strosio, *J. Appl. Phys.* 1998, vol. 84 No. 7, pp.3459-3466.
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1. "Modeling of Hot Acoustic Photon Propagation in Two Dimensional Layers," N. Bannov, V.V. Mitin, and F.T. Vasko, *VLSI DESIGN*, 1998, vol. 6, No1-4, pp.

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1. "Acoustic Phonon Modulation of the Electron Response in Tunnel-coupled Quantum Wells," F.T. Vasko and V.V. Mitin, Phys. Rev. B, 1997, Vol. 56, No. 23, pp. 15224-15230.
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*Papers presented at meetings, but not published in conference proceedings:*

1. "Optimization of Superconducting Hot-Electron Sensors: Controlling of Electron-Phonon Relaxation," A. Sergeev and V. Mitin, 11<sup>th</sup> International Symposium on Space Terahertz Technology, May 1-3, 2000, Ann Arbor, MI, book of abstracts, Session 7.
1. "Controllable Electron-Phonon Dephasing and Relaxation in Superconducting Qubits", V. Mitin, A. Sergeev, 11<sup>th</sup> International Winterschool on New Developments in Solid State Physics: Low-Dimensional Systems: Fundamentals and Applications, February 21-25, 2000, Mauterndorf, Austria.
1. "Effect of Boundaries and Impurities on Electron-Phonon Dephasing", A. Sergeev and V. Mitin, Surfaces and Interfaces of Mesoscopic Devices, Maui, Hawaii, December 5-10, 1999, Session 6.
1. "Contribution of Effective Mass Variations to Electron- Acoustic Phonon Interaction in Semiconductor Nanostructures", V. V. Mitin, V.I. Pipa, and, M. A. Strosio, The Forth International Symposium on New Phenomena in Mesoscopic Structures (NPMS'98), Dec. 6- 11, 1998, Kauai, Hawaii.



1. "Electron- Acoustic Phonon Interaction Via Deformation Potential in Semiconductors Nanostructures", Vladimir Mitin, Advanced Heterostructure Workshop 1998, Nov. 29- Dec. 4 1998, Kohala Coast Hawaii.
1. "Relaxation Rates of 2D Electron Gas Due to Near-Surface Acoustic Phonon Scattering" N. Z. Vagidov, V. I. Pipa and V. V. Mitin. 9<sup>th</sup> International conference on Phonon Scattering in Condensed Matter, 26-31 July 1998, Lancaster, England, book of abstracts, pp. EP 1-3.
1. "Influence of Hot-phonon Effects on Electron Relaxation in a GaAs/AlGaAs Quantum Cascade Laser Structure", G. Paulavicius, V. Mitin, and M.A. Strosio, American Physical Society Meeting, March 16-20, 1998, Los Angeles, CA., Bulletin of the American Physical Society, 1998, Vol. 43, No. 1, p. 304.
1. "Influence of the Heterostructure Surface on the Relaxation Rate of 2D-electrons", V. Mitin, Workshop on Surfaces and Interfaces of Mesoscopic Devices, Kaanapali, HA, December 7-12, 1997, Tu3.3.
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1. "Acoustic Phonon Modulation of the Electron Response in Tunnel-Coupled Quantum Wells," G. Kis, F. Vasko, and V. Mitin, Fifth International Workshop on Computational Electronics, Notre Dame, Indiana, May 28-30, 1997, p. P48.
1. "Interaction of 2D Electrons with Acoustic Phonons near the Semiconductor Surface and its Effect on 2D Electron Transport," B. Glavin, V. Pipa, V. Mitin, and M. Strosio, Fifth International Workshop on Computational Electronics, Notre Dame, Indiana, May 28-30, 1997, p. P47.
1. "Heat Dissipation from Quantum Structures," V. Mitin, G. Paulavicius, N. Bannov, and M.A. Strosio, Fifth International Workshop on Computational Electronics, Notre Dame, Indiana, May 28-30, 1997, p. WeP6.
1. "The effect of the Surface on the Transport Properties of 2D Electrons Interacting with Acoustic Phonons," V. Mitin, V. Pipa, F. Vasko, and B. Glavin. Presented at the Second International Conference on Low Dimensional Structures and Devices, Lisbon, Portugal, 19-21 May 1997.
1. "2D Electron Mobility Dependence on the Position of a Quantum Well Within a Slab", M. Strosio, V. Pipa, B. Glavin, Vladimir Mitin, American Physical Society Meeting, March 17-21, 1997, Kansas City, MO., Bulletin of the American Physical Society, 1997, Vol. 42, No. 1, p. 678.

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## 7. Scientific personal

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1. Mitin V., Professor;
1. Korshak O., Research Associate;
1. Romanov D., Research Associate;
1. Glavin B., Research Associate;
1. Sergeev A., Research Associate;
1. Vagidov N, graduate student.

Working on this project, N. Vagidov has completed his is Ph.D. dissertation that he will defend in two months.